Annual Report to ONR

Project Title: Modeling the dispersion of vapor and aerosol particulates in the atmospheric boundary layer

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1. Introduction

When dealing with dispersion modeling in topographically complex surroundings there are several aspects to be considered. Does the topography give rise to preferred flow patterns, sea and land breeze cycles, mountain and valley winds, canalizations, etc.? When developing operational models there is also the question of available computer capacity. The selection of measurement locations in complex terrain, frequency of sampling, and selection of synoptic situations always place limits on the completeness of information about local flows. Observational studies provide useful information about the structure of parameters such as wind speed and direction, temperature, and humidity. However, one of the most critical issues is the structure of turbulence, which varies greatly over space and time in complex terrain and requires a great number of routine measurements to characterize. Determination of the turbulent transfer is essential to understanding and predicting the dispersion of atmospheric pollutants. Mountain flows are generally nonlinear and fully three-dimensional phenomena, and analytical models are applicable only to simple cases. In the present project, comparison of different dispersion models – a semi-Gaussian trajectory model and a higher-order closure dispersion model – will be performed. The observed or numerically simulated, by different dynamic models, wind, temperature, and turbulence fields will be used as inputs to these dispersion models. When choosing a modeling system, or combination of dynamic model and dispersion model, it is important to take into consideration the purpose of the simulations. If it is important to get good agreement between measurements and simulations for short-term sampling periods, a more complex modeling system needs to be used than if one is only interested in monthly, seasonally, or yearly mean values.

Local circulation over complex terrain is influenced by features such as differential heating of the ground and surrounding air, surface characteristics (vegetation, moisture and water coverage, roughness), large scale synoptic forcing, radiation, and clouds. However, one of the most significant determinants is topographic forcing of boundary-layer flow which creates a modification of stability, turbulence and the dispersion of atmospheric pollutants over complex terrain. In simulating the dynamics in complex terrain, it is not only important to study the influence of the surface characteristics etc., but also the grid resolution needed to resolve the most important topographic influence on the flow.

In comparison of simulated result with measured data one has to take into consideration the complexity of the area. If there are few sites with measurements – the most common

situation – and measurements are performed mostly close to the ground, a direct comparison between measurement and simulation is of very little use as a measure of a modeling system's capability to simulate the most apparent characteristics of the dispersion pattern in a specific area in complex terrain.

Usually one examines model simulations with measured data by statistically examining the agreement between measured and simulated data. Perhaps a better method to examine a model's consistency with "reality" is to determine a measure of a modeling system's disagreement to the measured data. For example this can be performed by calculating the distance in space where measurements and simulations agree with each other. As an example we can suppose we have an uplifted point source and that the plume passes a measuring site that shows a concentration value. However, the simulated plume does not reach the surface – either because of an underestimated vertical dispersion or an overestimated plume rise. The measured concentration value at surface is thus, in this example, simulated at a height of 20 m above the surface. Such a modeling system should be classified above a modeling system where the plume goes in an opposite direction, even though both systems give zero concentration value at the measuring site. In this project we will therefore introduce a different way of comparing measured and simulated concentrations. Furthermore, we will look at simulated concentration fields for different mean value periods to discover if simpler models can be used for long mean value periods.

2. Model Description

In this project we will test two different dispersion models and four different models that provide the dispersion models with meteorological data. The two dispersion models are of different complexity. The first is a so-called higher-order closure model that is very computer demanding and time consuming, especially when used for point sources. That model should therefore only be used for special investigations in the case of point sources. In this project we will use it for a short simulation period during the summer intensive study. As it needs all the second moments from a dynamic model, only a higher-order closure dynamic model (in our case the MIUU-model, see below) can be used as a data creator to the higher-order closure dispersion model. The second one is a semi-Gaussian trajectory model that calculates trajectories from the point source by using the wind fields simulated with different dynamic models. The dispersion around these trajectories is calculated by using a Gaussian distribution.

2.1 Higher-order closure dispersion model

The higher-order closure dispersion model (HOCD) solves prognostically the mean concentration of atmospheric pollutants, as well as the second-order moments that include fluctuating concentration. The model is a Eulerian diffusion model with the mean concentration equation (in tensor notation):

$$\frac{d\overline{C}}{dt} = -\frac{\partial \overline{u'_i c'}}{\partial x_i}. \qquad (1)$$

The corresponding equations for the turbulence fluxes are:

$$\frac{d\overline{u'_i c}}{dt} = -\overline{u'_i u'_j}\frac{\partial \overline{C}}{\partial x_i} - \overline{u'_j c'}\frac{\partial \overline{U_i}}{\partial x_j} - \frac{2}{3}\frac{g_i}{\overline{\Theta}_0}\overline{c'\theta'} + a_3\frac{\partial}{\partial x_3}q\lambda\frac{\partial \overline{u'_i c'}}{\partial x_3} - \frac{\alpha_3 q}{\lambda}\overline{u'_i c'} \quad , \qquad (2)$$

and the equation for the covariance between concentration and potential temperature is

$$\frac{d\overline{c'\theta'}}{dt} = -\overline{u'_j \theta'}\frac{\partial \overline{C}}{\partial x_j} - \overline{u'_j c'}\frac{\partial \overline{\Theta}}{\partial x_j} + \alpha_4\frac{\partial}{\partial x_3}q\lambda\frac{\partial \overline{c'\theta'}}{\partial x_3} - \frac{\alpha_3 q}{\lambda}\overline{c'\theta'} \quad , \qquad (3)$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \overline{U_i}\frac{\partial}{\partial x_i} \quad ;$$

$\overline{C}$ is the mean concentration; c' is the fluctuating part of the mean concentration; g_i is the acceleration of gravity; $g_i = (0, 0, -g)$; q^2 is the twice the turbulent kinetic energy; $\overline{U}$, $\overline{V}$, and $\overline{W}$ are the mean wind components in the x, y, and z-directions, respectively; u'_i is the fluctuating part of the wind component in tensor form; $\overline{\Theta}$ is the mean potential temperature; θ' is the fluctuating part of the potential temperature; and λ is the turbulent length scale. More detailed information on the dispersion model and the closure constants is given by Enger (1986, 1990).

The HOCD model is a Eulerian diffusion model that solves the dispersion in a polar coordinate system with its origin at the source in order to get a denser grid close to the source (Enger and Koracin, 1995, hereafter referred to as EK95). In the present study a simplified version of the model is used. Only the mean concentration equation is solved prognostically; the fluxes are derived by analytical expressions derived by assuming locally horizontally homogeneous meteorological fields and that the tendency and diffusion terms in the equations for the fluxes are negligible.

A terrain-following coordinate system is used in the vertical to introduce the topography in the model. The separation between the grid points in the vertical coordinate is smallest at the source height, where it is set to be 15 m. Forty-three (43) grid points up to 3000 m have been used in the vertical direction. In the horizontal polar coordinate system 181 grid points have been used in the angular direction. An equally spaced grid has been used providing a resolution of 2° between the grid points. A variable grid is applied in the radial direction, with the smallest grid distance closest to the source (about 500 m). Fifty-one (51) grid points have been used in the radial direction and the outermost grid point is 145 km from the source. The advection is solved by using an upstream scheme that has been corrected for numerical diffusion (Enger and Grisogono, 1998). Comparison of simulated concentrations and measured data by using the HOCD model is reported in Enger (1986), Enger (1990) and EK95.

2.2 *Gaussian trajectory dispersion model*

Enger and Koracin (1995) demonstrated that a higher-order dispersion model was able to predict a detailed structure of SO_2 concentrations and that the results compared well with surface and aircraft measurements. Since this higher-order closure model is fairly complex and the computational time is even longer than the fully prognostic atmospheric model, it is not practical for longer-term (week-month-year) dispersion calculations. Therefore, a semi-Gaussian, trajectory-type dispersion model (SGTD), which is more suitable for longer-term dispersion estimates are tested as well. The model calculates trajectories for the plume from the simulated wind fields and approximates the concentration fields with a bi-Gaussian distribution. Since the concentration field at a certain time will be built up of several trajectories, a Gaussian distribution of the concentration around a trajectory does not mean that the concentration field must look Gaussian.

There are a wealth of σ_y and σ_z formulas available in literature. Algorithms for $\sigma_{y,z}$ can generally be divided into three groups: methods based on power law functions (e.g., Briggs, 1974, classical interpolation formulas), methods based on statistical parameters, such as horizontal and vertical direction variances (e.g., Draxler, 1976), and methods based on similarity theory (e.g., Berkowicz et al. 1985). With standard deviation formulas for the lateral spread (σ_y) as proposed by Briggs (1974), Draxler (1976) or Berkowicz et al. (1985), it appears that the measured lateral spread increases faster downwind in a complex terrain area than is predicted by ordinary $\sigma_y(x)$-algorithms, see Andren (1987). This might be due to wind direction shear in the vertical, a problem that was first treated by Hogstrom (1964). Smith (1965) presented a method that explicitly deals with this effect by extending Hogstrom's result to spectral representation. The derivation was made for the case of a passive tracer in a field of homogeneous turbulence and constant wind direction shear. Transforming Smith's result into an Eulerian framework, using the hypothesis $(T_L/T_E)_{v,w} = \beta_{v,w} = C/i_{v,w}$, where T_L and T_E are Lagrangian and Eulerian time scales and $i_{v,w}$ is turbulence intensity, gives the vertical standard deviation:

$$\sigma_z^2 = \sigma_w^2 t^2 \int_0^\infty F_{Ew}(n) \left[\frac{\sin^2\left(\frac{\pi n t}{\beta}\right)}{\left(\frac{\pi n t}{\beta}\right)^2} \right] \left[1 - \frac{\sin^2\left(\frac{\pi n T_s}{\beta}\right)}{\left(\frac{\pi n T_s}{\beta}\right)^2} \right] dn \,, \tag{4}$$

and the lateral standard deviation:

$$\sigma_y^2 = \sigma_v^2 t^2 \int_0^\infty \left(F_{Ev}(n) - \left(\frac{v_*^2}{\sigma_v \sigma_w}\right)^2 F_{Ew}(n) \right) \left[\frac{\sin\frac{\pi n t}{\beta}}{\frac{\pi n t}{\beta}} \right]^2 \left[1 - \left(\frac{\sin\frac{\pi n T_s}{\beta}}{\frac{\pi n T_s}{\beta}} \right)^2 \right] dn$$

$$+\frac{1}{4}\sigma_w^2\left(\frac{\partial V}{\partial z}\right)^2 t^4 \int_0^\infty F_{Ew}(n)\left[\frac{\sin\frac{\pi nt}{\beta}-\frac{\pi nt}{\beta}\cos\frac{\pi nt}{\beta}}{\left(\frac{\pi nt}{\beta}\right)^2}\right]^2\left[1-\left(\frac{\sin\frac{\pi nT_s}{\beta}}{\frac{\pi nT_s}{\beta}}\right)^2\right]dn\,, \qquad (5)$$

where F_{Ev} and F_{Ew} are normalized Eulerian energy spectra for lateral and vertical velocity components, respectively. σ_v^2 is the variance of Eulerian velocity fluctuations in the lateral direction, σ_w^2 is the variance of Eulerian velocity fluctuations in the vertical direction, and $v_*^2 = -\overline{v'w'}$. The expressions within brackets containing sine-functions are sine-function filters. One of the filter-expressions effectively filters out turbulence fluctuations with time scales greater than the sampling time, T_s, and the other one with time scales less than the travel time, t. The constant C has, by various authors, been given values between 0.35 and 0.8. In this study a value of 0.6 has been used. For the turbulent energy spectra, the analytical expression obtained from fitting the experimentally measured spectra have been used, see Enger (1983) and Andren (1987).

The wind direction shear not only influences the relative lateral spread but also affects the position of the plume centerline. Wind direction shear can generally be large in the studied area, which means that the plume can split and proceed in different directions. One simple way to take this effect into consideration is to calculate trajectories at different heights within the plume. In this study we have calculated trajectories at two heights, one for the center of mass of the plume and the other one for a height that is some distance below that height. We have chosen a level below the center of mass of the plume for the second trajectory, as wind direction changes are usually most pronounced closer to the surface. The choice of height for the second trajectory is quite ad hoc, and we have just chosen a height that is 0.5 σ_z below the center of mass of the plume. Furthermore, half of the emission mass from the point source is supposed to follow the center of mass of the plume and half to follow the lower trajectory. Trajectories and travel (aging) time are calculated for plume releases from the point sources at an interval of 5 minutes. Hourly concentrations at a certain point are calculated using all released parcels that are reaching that grid point within the specific time period.

2.3 The mesoscale meteorological models

Different sets of wind and turbulence fields characterized by differing complexities of atmospheric information were used as input to the dispersion calculations:

- Measured wind profiler data (WP wind fields)
- CALMEL, diagnostic model
- MM5, first-order closure model
- MIUU, second-order closure model

The first set was obtained by interpolation and extrapolation of data measured by wind profilers at MOHAVE Power Project (MPP or MOPP), Meadview (MEAD), Overton

Beach (OVBE), and Truxton (TRUX). The profilers were located within the range of 150-200 km around the source. The measurement data were interpolated and extrapolated for a 300 by 300 km^2 domain with a resolution of 3 km between grid points.

The second set was derived from the diagnostic atmospheric model CALMET (Scire et al., 1995) and will be indicated as CALMET fields. CALMET produces gridded fields of wind components, mixing heights, stability categories, micrometeorological parameters, and precipitation. The model uses standard hourly surface and twice-daily upper air observations as input. It can also use specially collected meteorological data such as hourly radar wind profiler data or a combination of various types of data. CALMET can also use outputs from different atmospheric models such as MM5 as inputs. In our case upper air data from three wind profilers located at MPP, MEAD, and TRUX were used as inputs for the CALMET simulation (Vimont, 1997). The model was run with a domain of 300 km west-east by 400 km south-north, using a spatial resolution of 5 km. Wind fields were simulated at 12 vertical levels from the surface to 3 km AGL.

The third set, referred to as MM5 wind fields, was obtained for a limited period, Julian days 219 through 226, 1992. The MM5 model was developed by the National Center for Atmospheric Research and the Pennsylvania State University (Grell et al., 1995). Since the late 1970s, this model has been used in many studies of regional and mesoscale weather phenomena. Mesoscale Model 5 preprocessing includes an advanced objective analysis of the synoptic data from the global network and provides detailed initial and boundary conditions for simulations. We used a non-hydrostatic version of MM5 with a 3 km horizontal resolution. The model domain consisted of 91 $\times$ 124 horizontal grid points and 35 vertical levels. The grid was centered at 35.7 N and 114.0 W. In order to include more upper-air measurements in the initialization process, an expanded grid of 60 km beyond the boundary of the model grid was used. Due to high horizontal and vertical resolution as well as a large number of grid points, the model required significant computational effort. Because of this limitation, only a selected episode from 7 through 14 August, 1992 was simulated by using MM5 over a specific domain.

The fourth set, referred to as the MIUU-model's wind and turbulence fields, is a non-linear, three-dimensional, hydrostatic, incompressible numerical modeling system with second-order closure that has been developed at Meteorological Institute Uppsala University (MIUU), Sweden during the last two decades. The modeling system consists of a number of nested models. The outermost model is driven by a synoptic model – in this study the model at the European Weather Center in England has been used. The inner models are driven by the same pressure fields and by employing the forcing of the mean values from the larger model at the boundaries. The dynamic models consist of prognostic equations for the horizontal wind components, liquid water potential temperature, mixing ratio of total water, and turbulence kinetic energy. The model is fully described and applied to the Colorado River Valley in Mohr and Enger (1999). Simulations have been performed for several nested models to receive wind and turbulence fields with different horizontal resolutions of 6 km, 3 km, and 1.5 km.

3. Simulation Domain

An extensive field program, the Measurements Of Haze And Visibility Experiment (MOHAVE), was conducted in winter and summer 1992 in the southwest U.S. The main objectives of the program were to investigate and identify the possible short- and long-term impacts of atmospheric pollutants from major urban areas and industrial sources on the Grand Canyon and its vicinity. A meteorological network of surface and upper-air stations was set up in the region to characterize atmospheric transport. The area is characterized by a complex topography of river and dry valleys as well as high plateaus.

4. Description of the Field Program

4.1 Measurements and tracer release

The field experiment performed in the area during 1992 was sponsored, designed and implemented as a partnership between the Environmental Protection Agency (EPA), Southern California Edison, and the National Park Service with technical support from a number of government, academic, and industrial organizations. The field study consisted of two intensive monitoring periods (January 4, 1992 to February 13, 1992 and July 7, 1992 to August 31, 1992), which included monitoring of PM2.5 aerosol and SO_2 at over thirty locations, optical monitoring at 10 locations, plus extensive augmentation of the surface and upper air meteorological monitoring throughout the region. The intensive monitoring periods also featured the continuous release from a few locations of perfluorocarbon compounds as tracers to investigate transport and dispersion. PFTs used in the Project MOHAVE are fully fluorinated hydrocarbons with low solubility in water and moderate vapor pressure that are therefore inert and non-depositing, as well as non-toxic. The PFT ortho-perfluorodimethylcyclohexane (oPDCH) was released continuously from the stack of MPP during the 30-day winter and 50-day summer intensive periods. Forty-five percent of the oPDCH consist of the isomer ortho-cis (ocPDCH), which has a background of about 0.52 parts per quadrillion (10^{-15}) or femtoliters per liter (fL/L). The tracer was released from the MPP stack at a rate proportional to the power production. The tracer release rate was constant when the power production stayed within 10% range of maximum load. For example, if power production was between 90% and 100% of capacity, oPDCH release rate were at their maximum and constant. If the power production dropped to between 40% and 50% of capacity, tracer release rates were reduced to one-half the maximum rate. For the summer, accurate SO_2 emissions measurements were not available; however the winter emissions monitoring showed a high correlation ($r^2 = 0.99$) of emissions with power production. Thus, power production is a good surrogate for SO_2 emission rate. For the summer, the ratio of power production to tracer release rate had a standard deviation of 6.9% and a r^2 of 0.83. The nearly constant ratio between tracer and SO_2 release allowed the calculation of the virtual amount of co-emitted sulfur associated with a given tracer concentration. This is the concentration of MPP sulfur that would be present in the absence of deposition and other atmospheric loss mechanisms. The full load of oPDCH emission rate was about 40 mg/s, which for two extended periods in the winter intensive and one in the summer intensive dropped to about half that rate. The emissions ratio R of

SO_2 to ocPDCH at MPP was maintained throughout the experiment such that the virtual concentration of 650 ng S/m^3 STP should accompany each 1 fL/L of ocPDCH. The average SO_2 to ocPDCH release ratio from MPP was 78.1 g SO_2/mg ocPDCH (488000 moles SO_2/mole ocPDCH) in winter and 73.3 g SO_2/mg ocPDCH (455000 moles SO_2/mole ocPDCH) during summer.

Table 1 shows the tracer sampling sites used in the present project together with the tracer release site (MOPP, which is the same as MPP).

Daily 24-hour duration samples starting at 7:00 MST at all sites, except at Meadview and Hopi Point, where twice daily 12-hour duration samples started at 7:00 MST and 19:00 MST, were collected using a Programmable Atmospheric Tracer Sampler (PATS). Sampling at most sites using the PATS was initiated at least 3 days prior to and continued at least 3 days after the PFT release periods. The PATS and PFT analyses techniques have been developed primarily at the Brookhaven National Laboratory (Dietz, 1996 and Draxler et al., 1991).

In addition to the 24- and 12-hour sampling, higher time resolution monitoring of PFTs was conducted for limited periods of time at the Meadview and Dolan Springs sites. A field version of the electron capture gas chromatograph with a dual trap (one sampling while the other is analyzed) was employed to collect and analyze on site the PFT concentrations with 15-minute time resolution for a two week period from July 28 to August 11, 1992 at the Meadview site. Occasional problems with the instrumentation caused by electric power interruption meant that this system was not operated continuously during this period. The Department of Energy collocated a PATS system programmed for two-hour sampling at the Dolan Springs site to take advantage of the nearby release of tracer at MPP as part of Project MOHAVE. This higher temporal resolution data is available from the DOE for a three-week period from July 9 to July 31, 1992.

Prior to the winter tracer study, a background study was performed to characterize ambient background tracer concentrations and their variability. PATS samplers were deployed at 27 sites for 10 days of twice daily 12-hour duration samples. Average background concentrations for each perfluorocarbon were calculated. For ocPDCH, one episode of elevated concentrations occurred at many sites during the background study. These elevated values were not used in the calculation of mean background. Calculated background concentration determined for the pre-test was ocPDCH, 0.52 fL/L. Sample volumes were not used to determine concentrations for the winter and summer study periods. Instead, the ratios of the chromatogram peak heights of each released PFT to ptPDCH (not released but analyzed and thought to be unchanging in the atmosphere) were compared to the ratios for the pre-release study period to calculate concentration. The background concentrations as determined for the three sampling periods prior to each of the two tracer release periods were slightly different from the separate background study:

Background study Nov 1991: 0.52 fL/L

Table 1. Tracer release (at MOPP) and tracer sampling sites used in the study.

Name	Lat	Long	Height ASL	Station Name
DOSP	35.5833	-114.2833	853	Dolan Springs, AZ
LVWA	36.1167	-114.8500	457	Las Vegas Wash, NV
MEAD	36.0222	-114.0675	905	Meadview, AZ
MOSP	35.9833	-115.5167	1753	Mountain Springs Summit, NV
OVBE	36.4333	-114.3667	396	Overton Beach, NV
SPMO	35.2500	-114.7333	1498	Spirit Mountain, NV
HOPO	36.0667	-112.1500	2164	Hopi Point, AZ
KING	35.2500	-114.0500	1040	Kingman, AZ
SQMO	35.2167	-113.1000	1981	Squaw Mountain, AZ
COCO	35.4833	-114.6833	274	Cottonwood Cove (West), NV
COCE	35.3472	-114.6655	201	Cottonwood Cove East, AZ
TRUX	35.4861	-113.5639	1350	Truxton, AZ
YUCC	34.7500	-114.1667	579	Yucca, AZ
MOPP	35.1453	-114.5906	213	MPP-Mohave power plant, NV
LOME	36.1000	-112.7000	1786	Long Mesa, AZ
SELI	35.2833	-112.4830	1661	Seligman, AZ
BAKE	35.2833	-116.0667	283	Baker, CA
BARS	34.9166	-116.9500	590	Barstow, CA
BRCA	37.6167	-112.1667	2438	Bryce Cancon, UT
NEHA	37.5000	-113.3000	1524	New Harmony, UT
KELS	34.8995	-115.6533	860	Kelso, CA
PARK	34.1500	-114.2667	137	Parker, AZ
ESSE	34.7500	-115.2500	520	Essex, CA
WICK	33.9333	-112.8000	732	Wickenburg, AZ
JOTR	34.0500	-116.2333	1250	Joshua Tree, CA
JALA	36.7000	-112.2167	2487	Jacob Lake, AZ
MACN	36.8000	-111.6500	1219	Marble Canyon, AZ
DARO	37.1333	-111.0500	1158	Dangling Rope
INGA	36.0833	-112.1167	1158	Indian Gardens,
ING5	36.0833	-112.1167	1158	Indian Gardens (12 Hour),
SYCA	35.1500	-111.9833	1890	Sycamore Canyon
TONT	33.6500	-111.1167	732	Tonto Nat. Forest
PAUL	34.9167	-112.5667	1341	Paulden,
AMBO	34.5625	-115.5458	213	Amboy,
DECE	33.7000	-115.3666	270	Desert Center,
SAGO	34.1933	-116.9133	1710	San Gorgonio Wilderness
HUMO	35.1167	-113.8667	2408	Hualapi Mountain
PEFO	34.9139	-109.7958	1690	Petrified Forest Nat. Park
TEHA	35.1000	-118.4333	1280	Tehachapi Summit
CAJO	34.3333	-117.4000	1076	Cajon Pass
CIBO	33.3000	-114.7000	72	Cibola Nwr

Winter study Jan-Feb 1992: 0.53 ± 0.05 fL/L
Summer study Jul-Aug 1992: 0.56 ± 0.06 fL/L.

The increase in calculated background between the background and summer studies was 8% for ocPDCH. It is expected that the true background values did not rise as much as 8%; rather, variability in the analytical methods and assumptions used in the concentration calculations are probably the reason for the increase.

Meteorological monitoring is necessary to characterize the speed, direction, and depth of air mass transport in the region and for model validation and initialization. The existing network of National Weather Service (NWS) and other monitoring sites in the region was insufficient to characterize the complex meteorological setting of the study area. Additionally, for the sparse network of NWS upper air measurement sites, vertical profiles were taken only twice per day. Thus, they did not capture potentially important changes in meteorological conditions, such as the full resolution of a diurnal cycle. While it was recognized that it would be impossible with available funds to set up a meteorological monitoring network to capture all flows of interest, the existing network was supplemented with additional measurement sites.

The additional sites had both surface and upper-air measurements. They consisted of Doppler wind profiling radars (915 MHz), Radio Acoustic Sounding Systems (RASS), Doppler sodars, and rawinsondes for upper air measurements and typically, wind speed and direction, temperature, relative humidity, and pressure for surface measurements. The radar wind profilers allow for continuous remote sensing of the three components of wind (u, v, and w) from about 100 m to 3-4 km or so above surface, with the maximum height being roughly proportional to absolute humidity. Data is reported as hourly averaged values of horizontal wind speed and direction and vertical velocity for 100 m thick layers at the high resolution mode and 400 m thick layers at the low resolution mode. At the higher levels, the 400 m mode provides greater data recovery than the 100 m mode. The RASS gives virtual temperature profiles by measuring the vertical distribution of the speed of sound using the scatter of radar waves from the vertically propagating acoustic waves (Neff, 1990). The RASS has a range of about 150 m to 600 m with a resolution of about 50 m.

The rawinsonde data of wind speed, wind direction, temperature, relative humidity (RH), and pressure from near the surface to 5000-6000 m AGL were used in this study. The resolution for wind speed and direction measurements was typically 50-100 m, while the resolution of temperature, RH, and pressure measurements was generally 20-30 m. The measurements were usually made twice per day, although measurements were also made three times per day. Surface meteorological measurements were also made at the optical monitoring sites and SCE's long-term air quality monitoring sites. Data from all National Weather Service monitoring sites in the study region were also archived and added to the Project MOHAVE database. During the summer, the US Army radiosondes at Yuma, normally used only 5 days per week, were augmented to 7 days per week. Although not sponsored by Project MOHAVE, additional radar wind profilers were also operated in

Southern California during the summer intensive study; data from three profilers is included in the Project MOHAVE database.

The following sites performed upper-air measurements during the summer intensive study:

MPP: WP, RASS, S
Truxton: WP, RASS
Meadview: WP, RASS
Overton Beach: S
Page: R
Cottonwood Cove, Dolan Springs: R

Where WP = Radar Wind Profiler, S = Sodar, R = Radiosonde, RASS = Radio Acoustic Sounding System.

4.2 Accuracy and precision of tracer measurements

It is important to know the accuracy and precision of the tracer measurements when we want to compare measured data with simulated ones. Use of collocated samplers was a key component of the quality assurance evaluation for Project MOHAVE tracer data. A previous perfluorocarbon tracer study performed by organization not involved with Project MOHAVE had collected tracer measurement results showing uncertainties in the tracer measurements larger than the highest concentration at the Grand Canyon receptor site (Richards et al., 1991); thus, demonstration of good precision using collocated samplers was critical for credibility of the Project MOHAVE tracer data. For both the winter and summer intensive periods, two locations (Meadview at the west edge of Grand Canyon National Park and Hopi Point near Grand Canyon Village) were chosen to have 3 tracer samplers each. Not only did this arrangement allow for calculation of collocated precision, it also provided for insurance at these key Grand Canyon monitoring sites in case of sampler failure. In addition to the collocated BATS (Brookhaven Atmospheric Tracer Sampler) samplers, the 15-minute real-time sampler at Meadview allowed for comparison with the BATS at Meadview for a portion of the summer period. The Environmental Monitoring Laboratory (EML) of the U.S. Department of Energy also made PFT measurements at one site (Dolan Springs); this data allowed comparison of the Brookhaven concentrations to a completely independent measurement. The EML study also had duplicate samplers, allowing for calculation of collocated precision for their measurements. Brookhaven National Laboratory was blinded to the locations of samplers, except by site number, as well as to which site number corresponded to collocated measurements.

Some problems were experienced in the collection of samples due to sampler malfunction and, in the summer, incorrect instructions given to site operators. In addition, a small percentage of the samples could not be indisputably assigned sampling times or locations.

Regression statistics (r^2, slope intercept, standard errors of slope, intercept, and y-estimate) were computed for each pairing of samplers and for each tracer compound during the summer and winter. Root-mean-square errors for winter and summer collocated PFT measurements at Meadview and Hopi Point are:

ocPDCH
Winter: RMSE = 0.021 (N = 279),
Summer: RMSE = 0.059 (N = 246).

Scatter-plots for collocated summer measurements of release tracer (ocPDCH) at Meadview show that there is a good precision for ocPDCH ($r^2 = 0.997$); this is especially important because the ocPDCH was used to tag the MPP emissions, the main source of interest for this study.

Collocated precision gives a measure of uncertainty in PFT concentrations over the range of concentrations experienced for two or more samplers at a given site. However, there may be additional uncertainty in the concentration of released PFTs due to variation in apparent background caused by a combination of actual variation in background and measurement error.

Because the average network-wide background PFT concentration was subtracted for each site, background that were constant at each site, but varying between sites would result in constant additive biases (systematic error) for each site. Background concentration varying in time at each site, but averaging the same at all sites would appear as random errors. For determination of PFT concentrations due to the release, the background variation calculation is preferred to collocated precision (especially at near background levels) because it includes both measurement error and actual variation background. At high concentrations of released tracer, collocated precision measurements more appropriately demonstrate multiplicative errors (e.g., slopes of regression analyses significantly different from one). When considering the amount of SO_2 associated with a given amount of ocPDCH released from MPP, the variation in the SO_2/ocPDCH emission rate must also be considered.

Standard deviations of the PFT compounds (pooled over all sites) during winter and summer pre-release periods and the interim period between the winter and summer studies are:

osPDCH winter standard deviation = 0.05 (N = 105),
summer standard deviation = 0.061 (N = 155),
Interim standard deviation = 0.037 (N = 83).

From July 28, 1992 through August 14, 1992 a gas chromatograph analyzed PFT concentrations for 15 minute sampling periods at Meadview. Although numerous power outages affected the overall data collection, a sufficient number of samples were collected to determine diurnal patterns of tracer concentrations as well as peak 15 minute to 12 hour average ratios, in particular for ocPDCH emitted from MPP stack. For each

12-hour averaging period the average of the 15-minute samples from the dual trap analyzer (DTA) was compared to concentrations from the Meadview 12-hour average sample from BATS. There were usually fewer than 48 valid 15-minute samples for comparison, so the actual sampling periods varied somewhat between DTA and BATS. The squared correlation coefficient (r^2) between the DTA and BATS was 0.79 (N = 30).

The Department of Energy's Environmental Monitoring Laboratory (DOE-EML) measured PFTs using the BATS samplers for 2-hour periods at Dolan Springs for the period July 11 – July 31, 1992. Dolan Springs is approximately 50 km north-northeast of MPP and was often expected to be in the transport path of MPP emissions during summer late-morning through afternoon periods. RMS error and r^2 for DOE-EML collocated tracer measurements at Dolan Springs:

ocPDCH RMS-error = 0.16 fL/L, r^2 = 0.98.

There were 14 days for which the EML PFT measurements could be compared to the Brookhaven PFT measurements at Dolan Springs. The 2-hour measurements from EML were averaged over 24 hour periods to compare with the BNL measurements. Most days had either 10 or 12 two-hour samples; several days were missing the 1600 and 1800 samples from EML. Time series plots comparing Brookhaven and DOE-EML concentrations show good agreement. Temporal patterns between Brookhaven and DOE-EML concentrations are similar for all PFTs (r^2 = 0.99 for ocPDCH). However, offsets are apparent for ocPDCH. The offsets indicate difference in apparent background values and do not affect concentrations due to release; thus the ocPDCH from MPP would not be affected by the offsets (about 0.1 fL/L).

4.3 Accuracy of upper-air wind speed and direction

Determination of the accuracy of the wind measurements is problematic because the "true" values are not known. However, comparisons of various measurement methods (e.g., rawinsondes, sodars, tall towers, radar wind profilers) and collocated precision calculations of a given method allow for a general level of uncertainty to be estimated. A review of routine field audits of radar wind profilers using rawinsondes, Doppler sodars, tethered-sonde systems, and pilot balloon tracking showed consistency of wind profiler measurements to within about 1-2 m/s in speed and 10 to 20 degrees in direction (Neff, 1994). Comparison of radar wind profiler observations to aircraft and tall tower measured wind indicated RMS differences of 1 m/s and 10 degrees (Angevine and MacPherson, 1996; Angevine et al., 1998). Guidelines for quality assurance of upper air meteorological data prepared for the USEPA give "expected" performance characteristics for radar wind profilers and rawinsondes (Lindsey et al., 1995). These guidelines give expected comparability for radar wind profilers of 2 m/s in speed and 30 degrees in direction, with systematic differences of 1 m/s and 10 degrees. The corresponding values for rawinsondes are 5-18 degrees in direction and 3.1 m/s in speed for comparability, based upon collocated precision, with systematic differences of 0.5-1 m/s for each component.

During about the first two weeks of the winter intensive study, a radar wind profiler (RWP) was located at MPP and rawinsondes were released nearby in the "Riviera" section of Bullhead City, AZ, about 4 km southwest of the RWP location. The height of the MPP RWP site and Bullhead City rawinsonde site were 213 m MSL and 167 m MSL, respectively. Although the instruments were nearby, they were not collocated, the reported measurement heights differed somewhat, and the RWP data were hourly averages while the rawinsonde data were nearly instantaneous. Nonetheless, comparison of the data from the two systems can give an upper limit on the measurement uncertainty of these instruments. Both the RWP and rawinsonde gave wind direction and speed approximately every 100 meters in height. For heights of about 400 m to 2700 m MSL, measurements from both systems were available for comparison. In order to compare values at the same height, the observations were linearly interpolated to the nearest 100 m.

Comparison of winds from rawinsonde and radar wind profiler:

Wind direction: percent within given direction differences:
10 degrees 50%, 20 degrees 78%, 30 degrees 94%;

Wind speed: percent within given speed differences:
1 m/s 41%, 2 m/s 63%, 4 m/s 84%;

Combined wind speed and direction: percent meeting both speed and direction criteria:
2 m/s and 20 degrees 52%, 4 m/s and 30 degrees 83%.

There was a bias of 5 degrees between the Bullhead City rawinsonde resultant wind direction and the MPP radar wind profiler resultant wind direction.

5. Comparison Method

Usually one examines model simulations with measured data by statistically examining the agreement between measured and simulated data. This will also be performed in this study for the different dispersion-meteorology modeling combinations. The comparisons will be performed for different long mean-value periods, from 1-day mean values up to entire intensive periods. The different model combinations are:

- HOCD-model + MIUU-model
- SGTD-model + MUII-model (3 different horizontal resolutions – 6 km, 3 km, and 1.5 km)
- SGTD-model + MM5-model (only for an eight days period during summer intensive)
- SGTD-model + CALMET-model
- SGDT-model + WP-data (from 4 wind profilers, see section 2.3)
- SGDT-model + wind profiler only at MPP.

Perhaps a better method of examining a model's consistency with "reality" is to designate a measure of a modeling system's disagreement with the measured data. A first check is

to examine if the plume is passing the measuring site (Index I_p) – either at surface or at a higher elevation. Another possible method is to calculate the distance in space where measurements and simulations agree with each other.

Index I_p	1	if plume above the measurement site and measured concentration > 0
Index I_p	$(\pi / 2 * R - \Delta s) / (\pi / 2 * R)$	if plume not above measurement site and measured concentration > 0

where R is the radius of a circle around the source, which is the distance between the source and a measuring site; and Δs is the distance on that circle between measuring site and the plume edge (concentration higher than a threshold value). This means that index I_p has values between –1 and +1, with value +1 if the plume passes the site and with value –1 if simulated plume goes in an opposite direction of the site.

Calculating the smallest distance between the observation point to a point below the simulated plume centerline height, which has the same concentration as the observed, gives three distances:

- Δs distance in angular direction
- Δr distance in radial direction
- Δz distance in vertical direction

from which we can define three indices: I_S, I_R, and I_Z.

Index $I_S = \Delta s / (\pi * R)$, with values between 0 (best agreement) and 1.

Index $I_R = \Delta r / R$, with values between 0 (best agreement) and 1.

Index $I_Z = \Delta z / Z_c$, where Z_c is the plume centerline height. Index I_Z has values between 0 (best agreement) and 1.

Furthermore, we will compare the different model combinations with each other by looking at the agreement or disagreement between the models by using statistics. The following statistical parameters will be calculated within a horizontal domain of 300 km × 250 km:

- Mean concentration at the surface for the whole domain
- Mean concentration integrated up to the top of the model for the whole domain
- Number of grid areas (1×1 km^2) with concentrations above a certain threshold at the surface

- Number of grid areas with concentrations above a certain threshold covered by both models at the surface
- Intersection area (area that is covered by both models in wither model).

The WP wind field, the CALMET fields, and the MM5 fields were obtained. The MIUU fields are underway. Dispersion works with these dynamic fields are also underway.

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